

Glycine ethyl ester
459-73-4 | DTXSID90196648

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 51.3 °C

Global applicability domain: Inside

Local applicability domain index: 4.42e-01

Confidence level: 5.54e-01

Nearest Neighbors from the Training Set

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Ethanamine, 2,2-diethoxy-

Measured: -78.0

Predicted: -53.9

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Thioacetamide

Measured: 116

Predicted: 113

Image not found

1-(2-Hydroxyethyl)pyrrolidin-2-one

Measured: 20.0

Predicted: 22.5

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Propanamide

Measured: 81.3

Predicted: 92.6

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Propanamide, 2-methyl-

Measured: 128

Predicted: 122